CHAPTER 6

A NEW COLLISION MODEL FOR POLYATOMIC MOLECULES

6.0 Introduction

In this chapter we present a collision model for polyatomic gases which may be considered to be intermediate between those that use a simple classical representation of the molecules and the statistical exchange schemes of Borgnakke and Larsen. The difficulty with the former approach is that it is not easy to devise simple classical models with the correct number of degrees of freedom. The rough sphere model, for example, is sufficiently simple but has three degrees of freedom for rotation. We propose that the energy exchange in collisions be calculated from a simplified, although rather abstract, representation of a collision. Any required number of degrees of freedom may be included but we present it for three translational and two internal degrees of freedom. Unlike the statistical exchange schemes, the post - collision 'state' is not selected from an equilibrium distribution for each collision but the equilibrium distribution is achieved for a large number of collisions.

The method is similar in some respects to the statistical schemes. An inelastic collision is defined in which energy is freely exchanged between internal and external energy and this may be used as part of a two class exchange scheme. The model may be easily extended to a restricted exchange scheme and has some computational advantages over the original methods when combined with a variable-ϕ equation. However, the method is not as versatile since in its basic form it only satisfies the detail balance condition for a Maxwell collision cross - section. The model can be used with any collision cross - section but to satisfy detail balance a slightly unsatisfactory modification must be made, which has little physical justification.

6.1 Equilibrium

Consider the equilibrium distribution of thermal velocities. The probability that a given molecule will have velocity in the range (v_1, v_2, v_3) to $(v_1 + dv_1, v_2 + dv_2, v_3 + dv_3)$ is

$$f(\underset{\sim}{v})\, dv_1\, dv_2\, dv_3 = \Phi(v_1)\, dv_1\, \Phi(v_2)\, dv_2\, \Phi(v_3)\, dv_3$$

where

$$\Phi(v_j) = \sqrt{\frac{m}{2\pi kT}}\, \exp(-mv_j^2/2kT).$$

Each component of thermal velocity is independently normally distributed. The Maxwell distribution is in fact the most probable distribution of velocities amongst the particles consistent with the conservation of the total energy. The proof, due to Jeans, applies to molecules with any internal structure for which the energy can be expressed as the sum of squared terms (Cowling 1950).

The method to be used in this collision model was suggested by Cowling's (1950, p. 104) interesting discussion of equipartition for a gas composed of N rotating rigid spheres having three degrees of translational freedom and three degrees of rotational freedom. He considers an 'equivalent' gas composed of 2N 'structureless' molecules having no internal energy. Half of these molecules have velocity components the same as the original molecules and the remainder have velocities such that their translational energy is equal to the rotational energy of a molecule in the original gas. The statistical theorems apply to this equivalent gas and he is able to deduce the rotational energy distribution in the original gas. In a similar manner we let each molecule have two internal energy components, v_j and v_k, which represent the rotational energy in each degree of freedom according to the rule

$$e_j = \tfrac{1}{2} m\, v_j^2 \qquad e_k = \tfrac{1}{2} m\, v_k^2$$

where $e_j + e_k$ is the total internal energy for one particle. The collision between molecules having translational and internal rotational energy will be represented by a collision in a five dimensional space between two ' pseudo particles' each having a five dimensional velocity representing the total energy. The statistical derivation of the equilibrium velocity and rotational energy distribution will still apply if these pseudo particles freely exchange energy in an arbitrary manner while conserving total energy.

By analogy with the monatomic collision in three dimensional velocity space we define the centre of mass velocity

$$v_{cm\ i} = \tfrac{1}{2}(v_i + v_i)$$

and the relative velocity of collision

$$g_i = (v_i - v_i)$$

in the five dimensional space (i = 1..5). The total energy of the two molecules is given by the same expression as in three dimensional space

$$\tfrac{1}{2} m \underset{\sim}{v}_{cm} \cdot \underset{\sim}{v}_{cm} + \tfrac{1}{4} m \underset{\sim}{g} \cdot \underset{\sim}{g}$$

and energy will be conserved if both $\underset{\sim}{v}_{cm}$ and $|\underset{\sim}{g}|$ are unchanged by the collision. The post- collision 'relative velocity' $\underset{\sim}{g}'$ will be the diameter of a 'hyper sphere' centered on $\underset{\sim}{v}_{cm}$. The post- collision 'velocity' points, which represent the state of the particles, cannot depart from $\underset{\sim}{v}_{cm}$ by more than $\tfrac{1}{2}\underset{\sim}{g}$ so there is a greater correlation between pre- and post- collision states than in the statistical exchange scheme. Perhaps more importantly the deflection angle in three dimensional space, which is a projection of the angle in five dimensional space between $\underset{\sim}{g}$ and $\underset{\sim}{g}'$, is linked to the amount of energy exchanged. Some sort of correlation like this exists for Parker's (1959) 'dumbell' molecule and it may be that this classical

collision in three dimensional space can be mimicked by the present model.

6.2 Geometry of 5 Dimensional Euclidean Space

The following geometrical results are required for this collision model. These are derived by analogy with three dimensional geometry. Cylindrical coordinates for an increasing number of dimensions are indicated in figure 6.1. The Cartesian coordinates of a point a distance r from the origin in 3 space are

$$\begin{aligned} x_1 &= r \cos\theta_1 \\ x_2 &= r \sin\theta_1 \cos\theta_2 && 0 < \theta_1 < \pi \\ x_3 &= r \sin\theta_1 \sin\theta_2 && 0 < \theta_2 < 2\pi \end{aligned} \qquad (6.1)$$

where r, θ_1 and θ_2 are the ~~cylindrical~~ spherical coordinates. In five space the Cartesian coordinates are

$$\begin{aligned} x_1 &= r \cos\theta_1 \\ x_2 &= r \sin\theta_1 \cos\theta_2 && 0 < \theta_1 < \pi \\ x_3 &= r \sin\theta_1 \sin\theta_2 \cos\theta_3 && 0 < \theta_2 < \pi \\ x_4 &= r \sin\theta_1 \sin\theta_2 \sin\theta_3 \cos\theta_4 && 0 < \theta_3 < \pi \\ x_5 &= r \sin\theta_1 \sin\theta_2 \sin\theta_3 \sin\theta_4 && 0 < \theta_4 < 2\pi \end{aligned} \qquad (6.2)$$

where r, θ_i , i = 1..4, are the 'hyper-~~cylindrical~~ spherical' coordinates.

The differential element of the area of the hyper sphere is

$$dA = r^2 \sin\theta_1 \, d\theta_1 \, d\theta_2 \qquad (6.3)$$

for three dimensions and

$$dA = r^4 \sin^3\theta_1 \, d\theta_1 \sin^2\theta_2 \, d\theta_2 \sin\theta_3 \, d\theta_3 \, d\theta_4 \qquad (6.4)$$

for five dimensions.

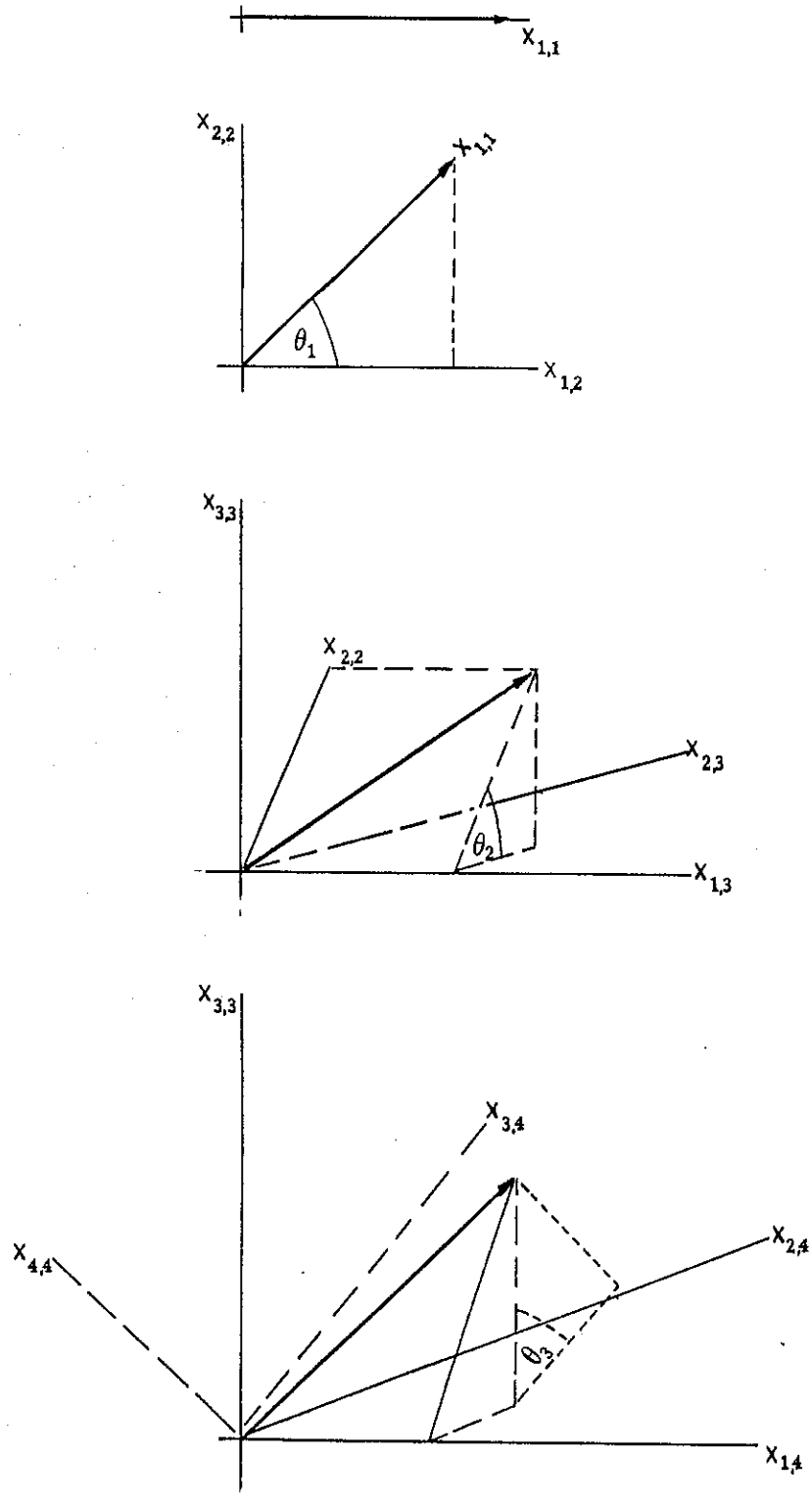


Fig. 6.1 ~~CYLINDRICAL~~ SPHERICAL COORDINATES FOR INCREASING NUMBER OF DIMENSIONS

6.3 Collision Model in 5 Space

The simplest collision model in the five dimensional space is an extension of the hard sphere collision in three dimensional space. For hard sphere collisions, given that the impact parameters are randomly selected, the components of $\underset{\sim}{g}'$ may be selected directly and the method is given by Bird (1976, p. 131). For a large number of collisions with velocity $\underset{\sim}{g}$ the end points of the vectors $\underset{\sim}{g}'$ are uniformly distributed over the surface of the sphere in velocity space. The number of post - collision relative velocity vectors with ~~cylindrical~~ coordinates θ_1 and θ_2 in the range θ_1 to $\theta_1 + d\theta_1$ and θ_2 to $\theta_2 + d\theta_2$ is therefore proportional to the elemental area $\sin\theta_1 \; d\theta_1 \; d\theta_2$. Defining the distribution functions f_1 and f_2 for the ~~cylindrical~~ spherical coordinates the number of these points in the elemental area is

$$f_1 \; d\theta_1 \; f_2 \; d\theta_2 = \sin\theta_1 \; d\theta_1 \; d\theta_2 .$$

The distribution of θ_2 is uniform so this coordinate can be selected directly from

$$\theta_2 = 2.0\,\pi \; R_f \qquad (6.5a)$$

The distribution of θ_1 is proportional to $\sin\theta_1$. Since $\sin\theta_1 \; d\theta_1 = -d(\cos\theta_1)$, the distribution of $\cos\theta_1$ is uniform and $\cos\theta_1$ may be selected directly from

$$\cos\theta_1 = 1.0 - 2.0\,R_f \qquad (6.5b)$$

The components of $\underset{\sim}{g}'$ are calculated from equations (6.1) with $r = g$.

In five dimensional space the components of $\underset{\sim}{g}'$ may be calculated similarly from an assumed uniform distribution of the direction of $\underset{\sim}{g}'$. The distribution functions for each of the 'hyper ~~cylindrical~~ spherical' coordinates are

$$f_1\ d\theta_1 \propto \sin^3\theta_1\ d\theta_1 \propto \sin^2\theta_1\ d(\cos\theta_1)$$

$$f_2\ d\theta_2 \propto \sin^2\theta_2\ d\theta_2 \propto \sin\theta_2\ d(\cos\theta_2)$$

$$f_3\ d\theta_3 \propto \sin\theta_3\ d\theta_3 \propto d(\cos\theta_3)$$

$$f_4\ d\theta_4 \propto d\theta_4.$$

The cosine of θ_1 is distributed proportional to $\sin^2\theta_1$ and the von Neumann technique is required to generate $\cos\theta_1$. The appropriate procedure is

repeat..

$$\cos\theta_1 := 1.0 - 2.0\ R_f$$

$$[\sin^2\theta_1] := 1.0 - \cos^2\theta_1$$

until.. $[\sin^2\theta_1] > R_f$. (6.5c)

The cosine of θ_2 is distributed proportional to $\sin\theta_2$ so the selection procedure is

repeat..

$$\cos\theta_2 := 1.0 - 2.0\ R_f$$

$$[\sin^2\theta_2] := 1.0 - \cos^2\theta_2$$

until.. $[\sin^2\theta_2] > (R_f)^2$. (6.5d)

The remaining coordinates θ_3 and θ_4 are selected in the same manner as in three dimensional space using equations (6.5a) and (6.5b). The five components of $\underset{\sim}{g}'$ are calculated from equations (6.2) with r = g. The final velocities and internal energies of both particles are determined from

$$\underset{\sim}{v}' = \underset{\sim}{v}_{cm} + \tfrac{1}{2}\underset{\sim}{g}'$$

$$\underset{\sim}{v}' = \underset{\sim}{v}_{cm} - \tfrac{1}{2}\underset{\sim}{g}' \qquad (6.6)$$

We can deduce the form of the 3 space scattering law which is incorporated into this model. Notice that if the coordinates i = 3 to 5 are the translational velocity components then the last three

equations of (6.2) have the same form as equations (6.1) with $r = g \sin\theta_1 \sin\theta_2$. In other words the deflection in three space is derived from the variable hard sphere collision dynamics with an altered relative velocity arising from the exchange of internal energy. The collision model can be combined with any scattering model in three dimensional space, whereby the deflection is calculated as usual from the pre- collision relative velocity and the randomly chosen impact parameters.

This collision model has been tested for stability and figure 6.2 shows a temperature history of a sample of 3000 particles. For simplicity a Maxwell cross - section was assumed so that pairs of molecules were selected for collision with equal probability independent of the relative velocity of collision. We later describe a modification which must be made if a different collision cross - section is used. It is not necessary to use time counters for these calculations and the time axis is marked in simulation collision time, i.e. collisions per particle, which can easily be converted to nominal collision time derived from viscosity by using equation (4.14). The initial velocity components (both translational and internal energy) were generated from the equilibrium distribution. Because of the finite sample size the initial translational temperature is about 2% greater than the equilibrium tempertaure, T_e, derived from the total energy but this difference was reduced by the action of collisions. This calculation was repeated a number of times and continued for up to 60 collision intervals. The translational temperature changed from above to below T_e many times and was usually within 1% and always within 2% of equilibrium.

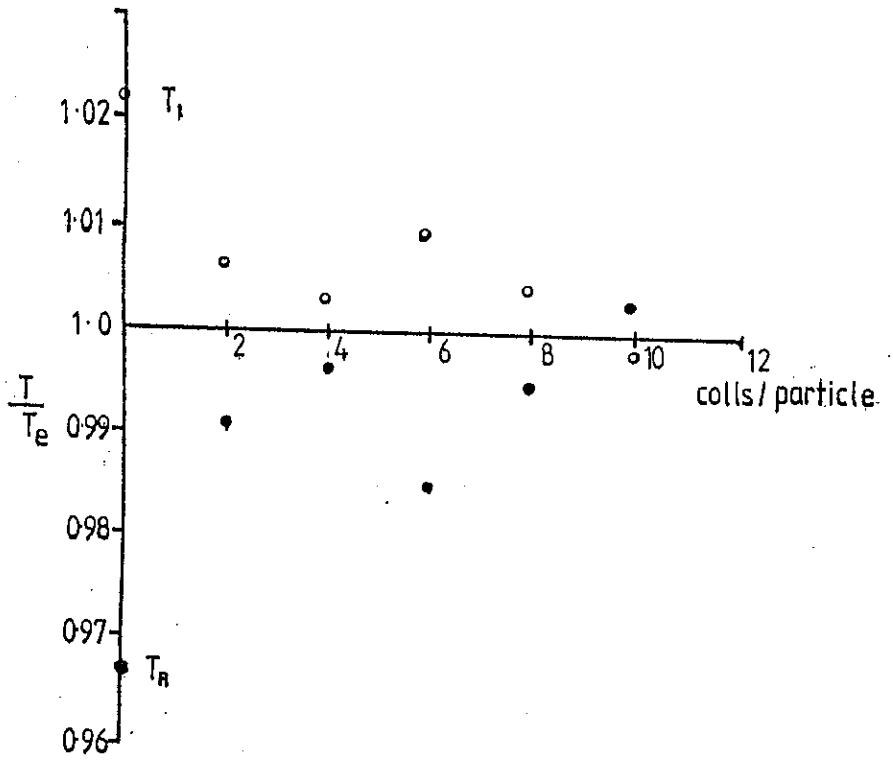
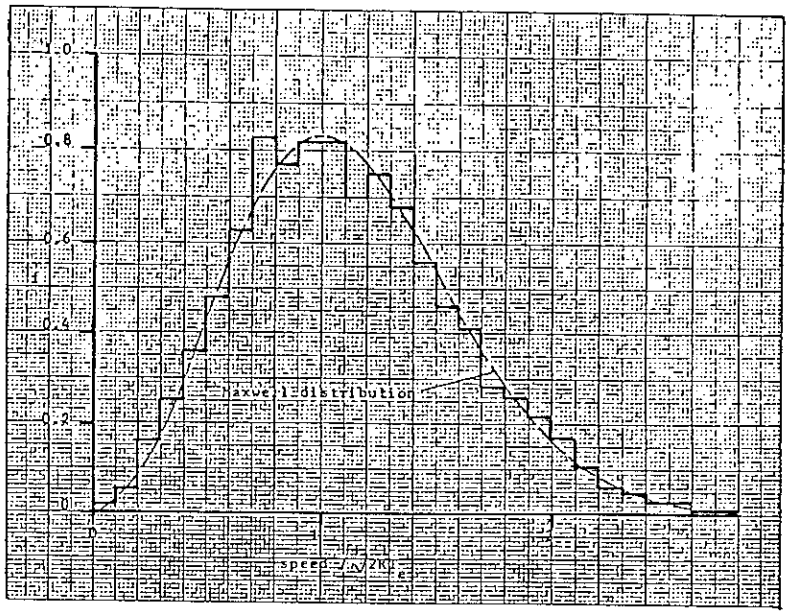


Figure 6.2 TEMPERATURE HISTORY : PSEUDO HARD SPHERE IN 5 SPACE

The distributions of speeds and internal energy after many collisions is compared with the theoretical distributions in figures 6.3 and 6.4. It is clear that the correct equilibriumdistributions are maintained. A similar stability test was made with the deflection angle in 3 space calculated using the LIP collision model described in chapter 4. These results are shown in figure 6.5 and are similar to those using hard sphere scattering.

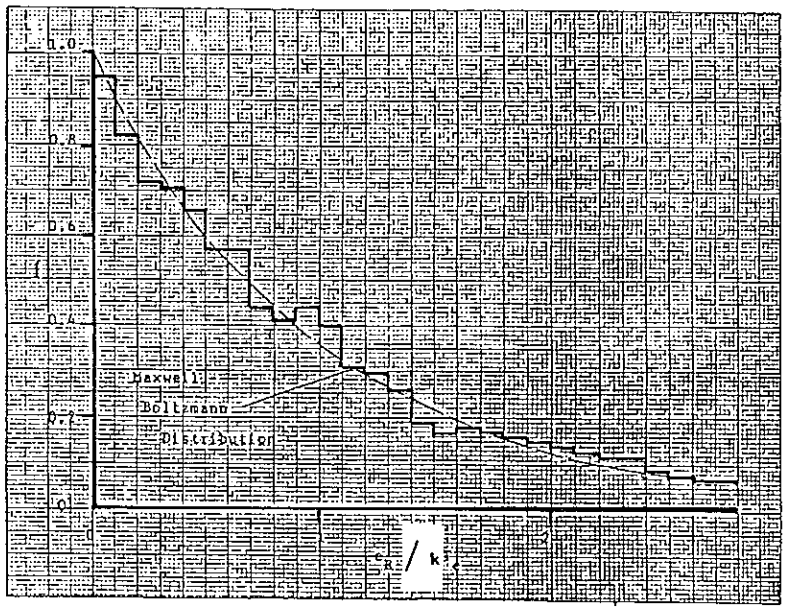
6.4 Restricted Exchange

It is easy in principle to restrict the amount of energy which is exchanged between internal and external modes in a collision. The



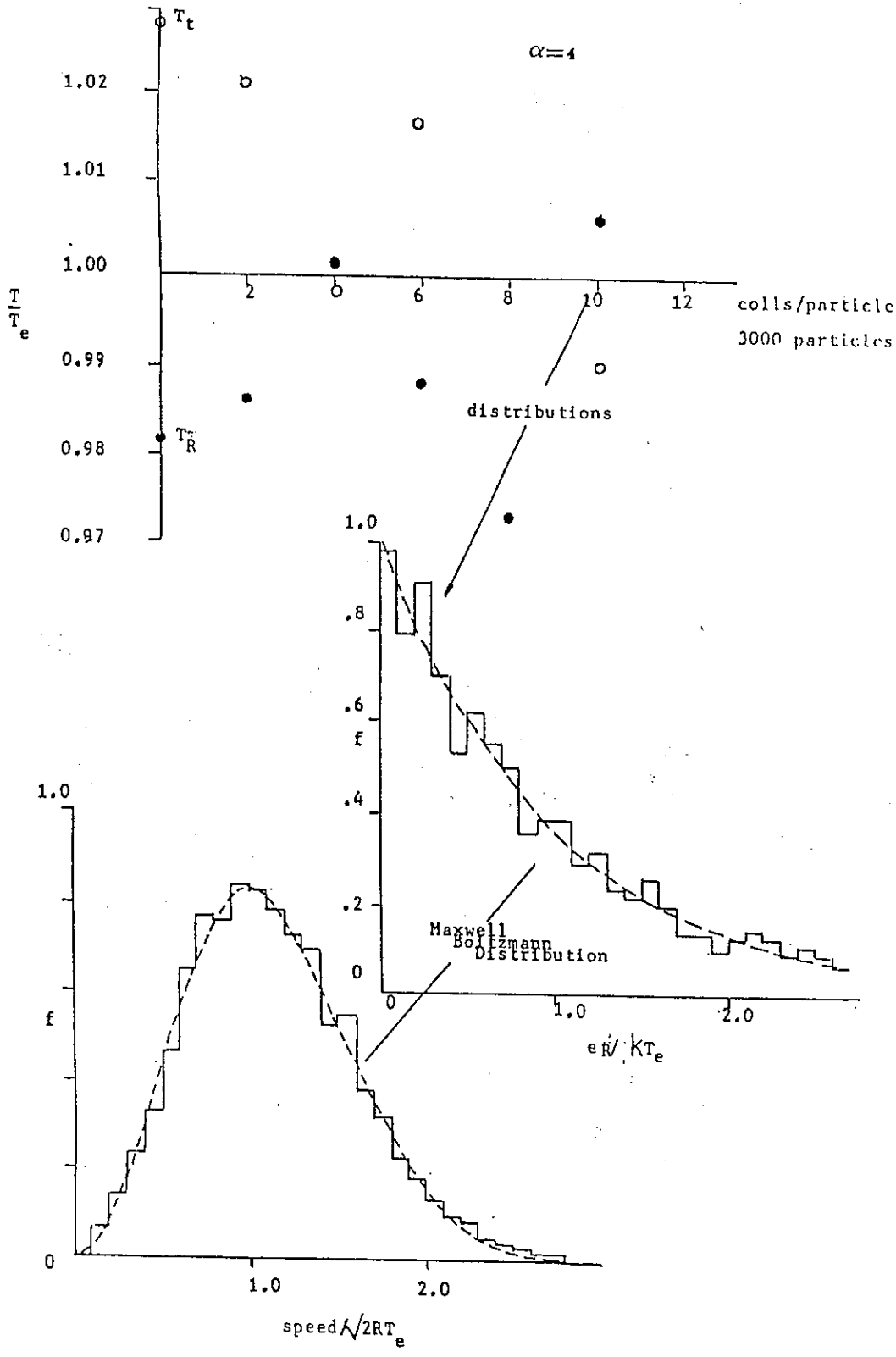
5-SPACE COLLISION MODEL : PSEUDO HARD SPHERE

Fig. 6.3 STABILITY TEST(a) MOLECULAR SPEED DISTRIBUTION



5-SPACE COLLISION MODEL : PSEUDO HARD SPHERE

Fig. 6.4 STABILITY TEST(a) INTERNAL ENERGY DISTRIBUTION

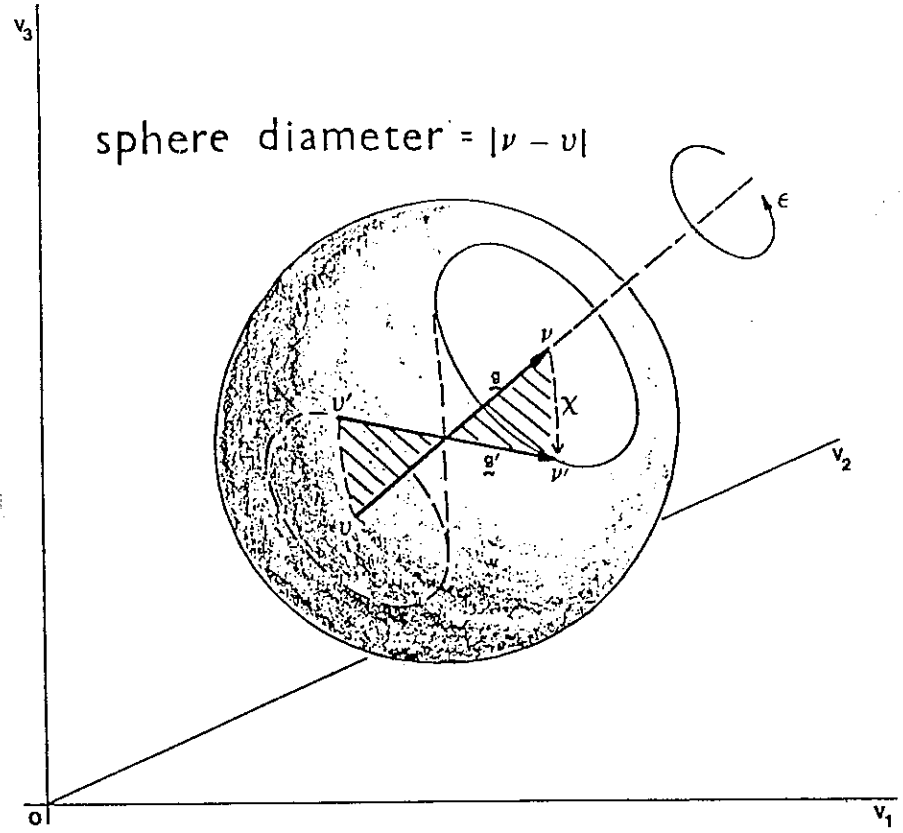


5-SPACE COLLISION MODEL

Fig. 6.5 STABILITY TEST(b) DEFLECTION FROM LIP MODEL

angle between the pre- and post- collision 5 vector g is the 'deflection angle in 5 space' and the greater this angle the greater will be the change in state across the collision. If this angle is limited to a value $\phi\pi$ the change in state is consequently limited.

It is useful to consider again the representation of a monatomic collision in three dimensional velocity space. If the deflection

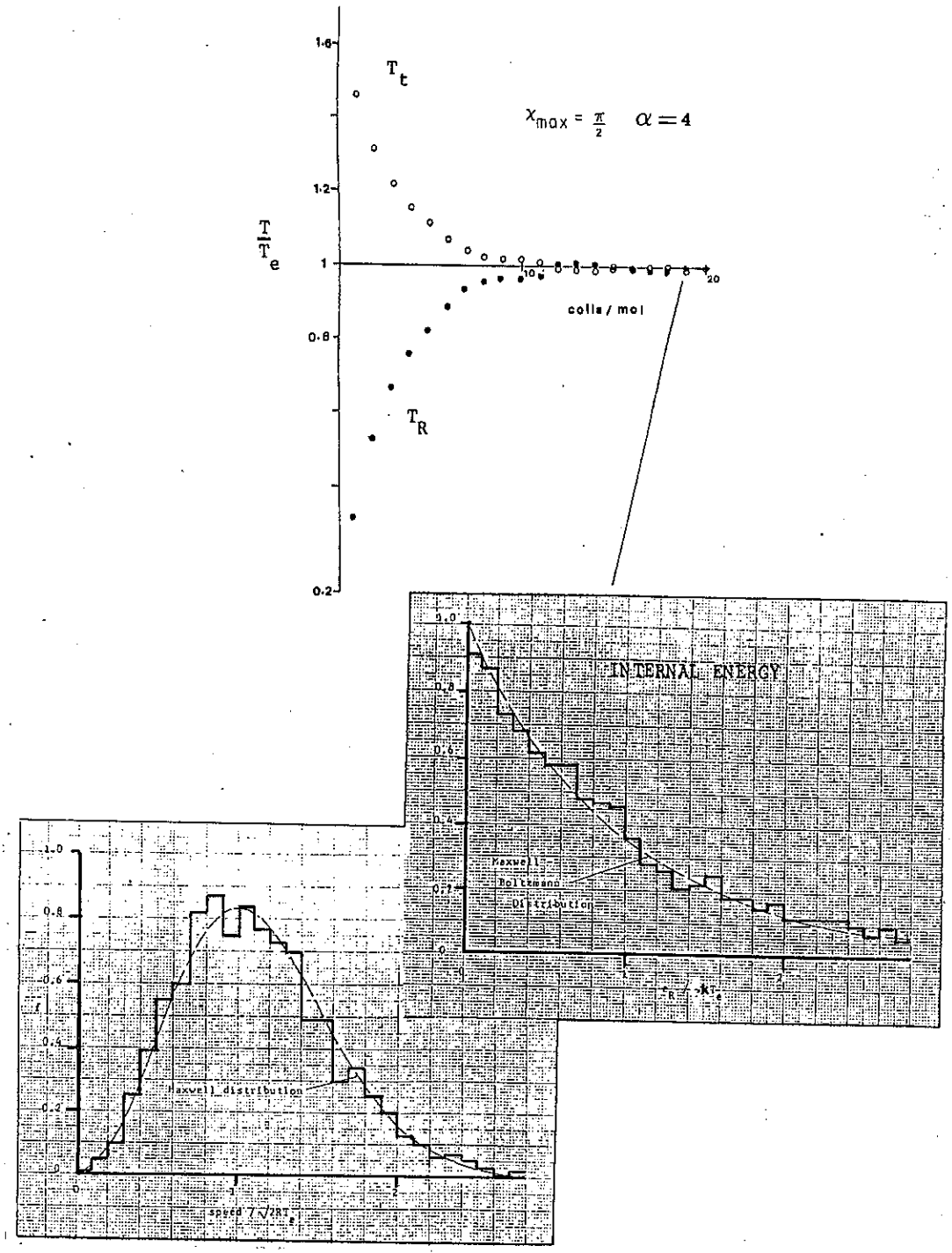


Collision in velocity 'space' $v\,u \rightarrow v'u'$

centre of mass velocity = $\frac{1}{2}(v + u)$

Figure 6.6 COLLISION IN VELOCITY SPACE

angle is limited, the direction of $\underset{\sim}{g}'$ must lie within a cone with half angle $\phi\pi$ and $\underset{\sim}{g}$ as the axis. The resulting distribution of post-collision velocity points on the surface of the sphere is axially symmetric about $\underset{\sim}{g}$. In five dimensional space the direction of $\underset{\sim}{g}'$ relative to $\underset{\sim}{g}$ is specified by the hyper cylindrical coordinates, g, θ_i (i = 2,3,4), selected from equation (6.6), and χ, where χ is the



VHS DEFLECTION IN THREE SPACE

Fig. 6.7 STABILITY TEST (c) 5-SPACE COLLISION MODEL: RESTRICTED EXCHANGE

restricted deflection angle $0 < \chi < \phi\pi$. The Cartesian components of $\underset{\sim}{g}'$ are then determined from these cylindrical coordinates and the orientation of $\underset{\sim}{g}$. The details are given in appendix C for three and five dimensions. The relaxation behaviour for ϕ = 0.5 is shown in figure 6.7 as well as the long time distributions of speeds and rotational energy. The scattering in 3 space was determined from the VHS model. The method works well and the equilbrium distribution is maintained.

6.5 Detail Balance

Unfortunately if the Maxwell cross - section is not used the method no longer satisfies the detail balance condition and equilibrium is not maintained. This is because the collision rates at different relative velocities are different for all but the Maxwell cross - section. The inverse of a collision with internal energy included has the same magnitude of the five dimensional 'relative velocity' vector (i.e. total energy) but not the same magnitude of the three dimensional relative velocity. Hence the inverse and forward collision rates are different. Detail balance can be satisfied if the collision probability depends on the magnitude of the 5 dimensional 'relative velocity' rather than the correct three dimensional velocity. In effect this adds a small perturbation, which depends on the internal energy, to the correct collision rate. Some classical models with internal energy behave in a similar, but not strictly analogous, way. For example, the different orientations of rotating dumb-bell molecules as they collide will produce slight variations in the collision cross - section and the 'correct' collision rate for these molecules is not as well defined as for simple representations of monatomic molecules. The least satisfactory aspect of using the five dimensional 'velocity'

when selecting pairs of particles for collisions is that particles with no relative velocity in 3 space might be chosen. The only possible, and admittedly slight, justification for this would be to suppose that the long range attractive force between two molecules initially at rest produced the collision.

The theoretical distribution of relative velocities in collisions at equilibrium depends on the variation of the collision cross - section. The distribution of the dimensionless collision energy $E = mg^2/4kT$ for inverse power cross - sections is

$$f_E \; dE = 1/\Gamma(2 - 2/\alpha) E^{1-2/\alpha} \exp(-E)\, dE \qquad (6.7)$$

(see Bird 1976, p. 184 for example). To determine how far the collision rate for the modified model departs from the monatomic

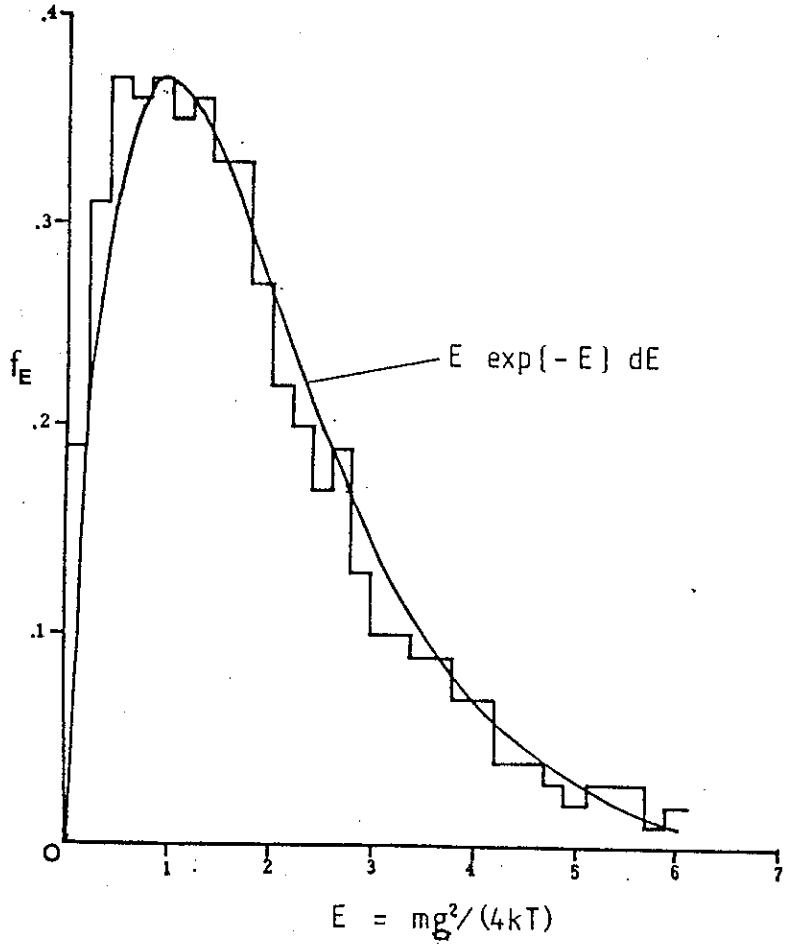
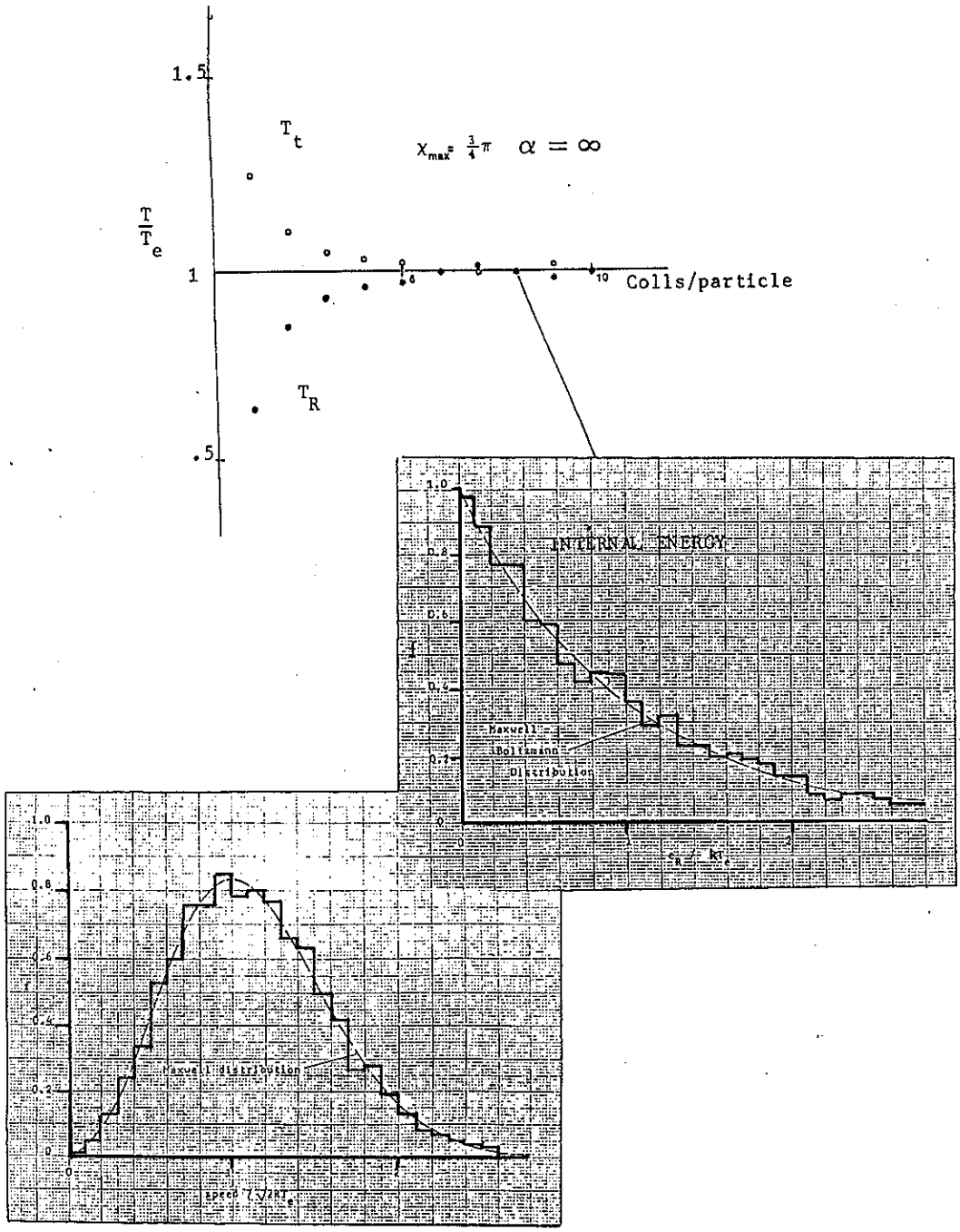


Figure 6.8 EQUILIBRIUM DISTRIBUTION OF COLLISION ENERGY IN SIMULATION

collision rate we have tested the collision model for hard sphere cross - sections ($\alpha = \infty$) where the relative probability of selecting a collision pair was made proportional to g in 5 space. The actual distribution of relative velocity in collisions using this modified collision probability was determined empirically from a simulation calculation and is compared with the correct distribution in figure 6.8. There is a slight shift in the relative frequencies towards the lower relative velocities but it does not appear to be a great distortion. Since the theoretical collision rate is derived from an idealised representation of the collision cross - section, it may be that this distortion of the relative collision rates is acceptable.

The relaxation behaviour with the modified collision probability is shown in figure 6.9. These results are better than for the Borgnakke and Larsen restricted exchange scheme which does not achieve detail balance (see for example Davis 1978, figure 29). It is possible that this 5-space model might be used in place of the restricted exchange scheme. When combined with a variable-ϕ equation the 5-space model executes 20% faster than the original scheme (see appendix D). This is in contrast to Pullin's (1978) modified restricted exchange which required twice as much machine time for each collision. However, a suggestion is given in appendix D which could make the original scheme up to 50% faster than the 5-space model with variable-ϕ. If this is so then the extra memory required for the 5-Space model (one element per particle) would certainly tip the balance in favour of the restricted exchange scheme, in spite of its small error in detail balance.



DEFLECTIONS FROM LIP MODEL

Fig. 6.9 STABILITY TEST (d): MODIFIED HARD SPHERE COLLISION PROBABILITY

APPENDIX C

FIVE SPACE COLLISION MODEL

The collision model in five space is derived as an extension of the methods used in three space. We first consider, in three space, how the components of $\underset{\sim}{g}'$ are calculated when $\underset{\sim}{g}$, the deflection angle and, ε, the orientation of the collision plane, are known.

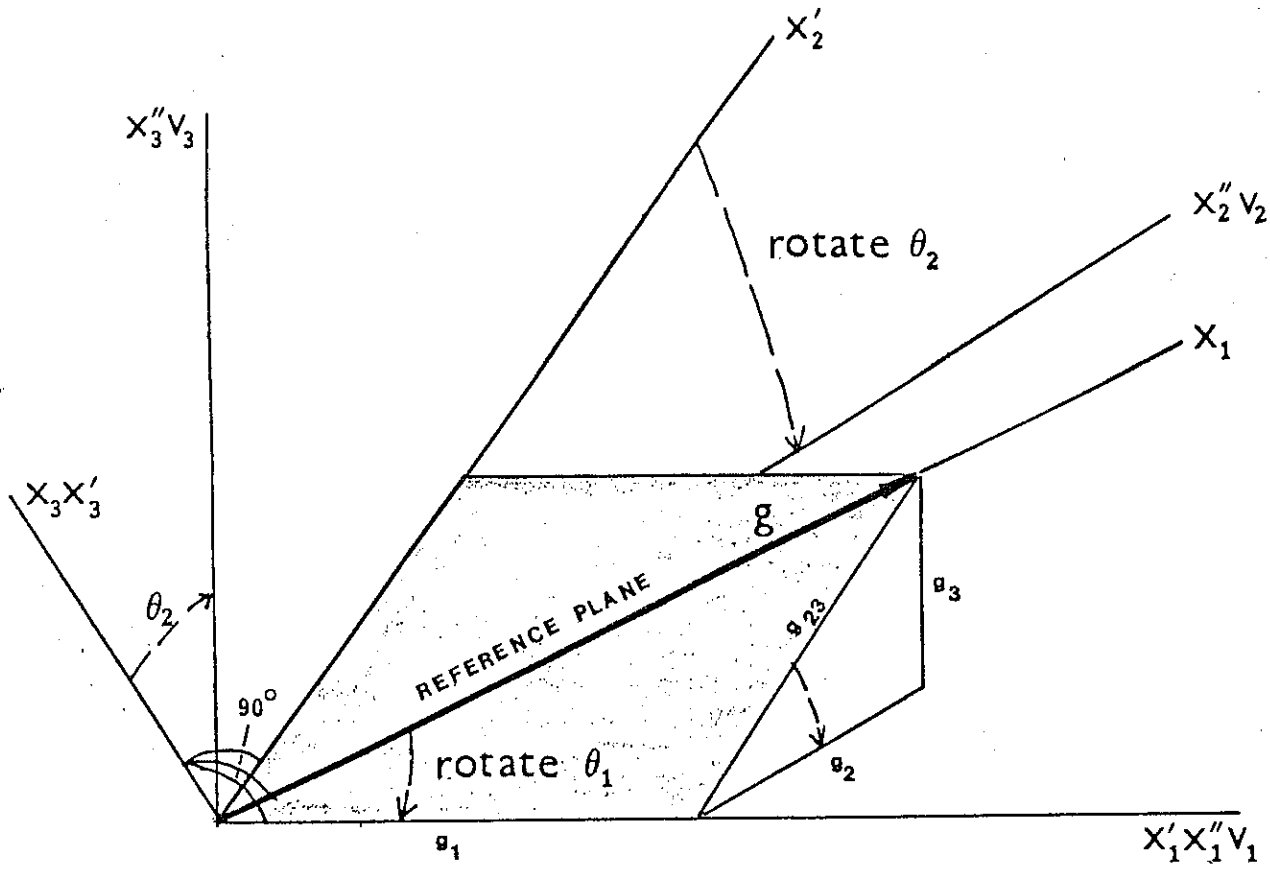


Fig. C.1 COLLISION COORDINATE SYSTEMS

Consider the Cartesian coordinate system (x_1, x_2, x_3) in velocity space (v_1, v_2, v_3) which is shown in figure C.1. The x_1 axis is directed along $\underset{\sim}{g}$ and the x_3 axis is perpendicular to plane containing $\underset{\sim}{v}_1$ and $\underset{\sim}{g}$, marked as the reference plane. The angle

ε is assumed to be measured from this plane. The cylindrical coordinates of $\underset{\sim}{g}'$ relative to (v_1, v_2, v_3) are g, θ_1, θ_2 where

$$\cos\theta_1 = g_1/g$$
$$\sin\theta_1 = g_{23}/g$$
$$\cos\theta_2 = g_2/g_{23}$$
$$\sin\theta_3 = g_1/g_{23} \qquad \text{(C.1)}$$

and where

$$g_{23} = (g_2^2 + g_3^2)^{\frac{1}{2}} .$$

The coordinate system (x_1, x_2, x_3) is transformed into the laboratory reference system (v_1, v_2, v_3) by two rotations:

(1) Rotation about the x_3 axis by an angle θ_1 until the x_1' and v_1 axes coincide, i.e.

$$\underset{\sim}{x}' = R\underset{\sim}{x}$$

where

$$\underset{\sim}{x}^T = (x_1\ x_2\ x_3)$$
$$\underset{\sim}{x}^T = (x_1'\ x_2'\ x_3')$$

and

$$R = \begin{bmatrix} \cos\theta_1 & -\sin\theta_1 & 0 \\ \sin\theta_1 & \cos\theta_1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

(2) Rotation about the x_1' axis by the angle θ_2 until x_2'' and x_3'' coincide with v_2 and v_3, i.e.

$$\underset{\sim}{v} = \underset{\sim}{x}'' = R'\underset{\sim}{x}'$$

where

$$\underset{\sim}{v}^T = (v_1\ v_2\ v_3) = (x_1'', x_2'', x_3'')$$

and

$$R' = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta_2 & -\sin\theta_2 \\ 0 & \sin\theta_2 & \cos\theta_2 \end{bmatrix}$$

The complete transformation is

$$\underset{\sim}{v} = R'R\underset{\sim}{x} . \qquad \text{(C.2)}$$

The cylindrical coordinates of $\underset{\sim}{g}'$ relative to (x_1, x_2, x_3) are g, χ and ε, the Cartesian components are

$$x_1 = g \cos\chi$$
$$x_2 = g \sin\chi \cos\varepsilon$$
$$x_3 = g \sin\chi \sin\varepsilon$$

and these may be substituted into equation (C.2) to give the components of $\underset{\sim}{g}'$ in the laboratory frame of reference.

In five dimensional space a similar transformation is required. The components of $\underset{\sim}{g}'$ relative to a coordinate system directed along $\underset{\sim}{g}$ are found from equations (6.2) as

$$\begin{aligned} x_5 &= g \cos\chi \\ x_4 &= g \sin\chi \cos\varepsilon_4 \\ x_3 &= g \sin\chi \sin\varepsilon_4 \cos\varepsilon_3 \\ x_2 &= g \sin\chi \sin\varepsilon_4 \sin\varepsilon_3 \cos\varepsilon_2 \\ x_1 &= g \sin\chi \sin\varepsilon_4 \sin\varepsilon_3 \sin\varepsilon_2 \end{aligned} \qquad \text{(C.3)}$$

where we have chosen for later convenience to renumber the axes from 5 down to 1. The angle χ is the restricted deflection angle chosen as

$$\chi = \phi\pi R_f$$

and the remaining angles (hyper orientation angles ε_i) are chosen so that the direction of $\underset{\sim}{g}'$ is isotropic within the hyper cone with half angle χ, i.e.

ε_4 is selected via equation (6.5d)

ε_3 is selected via equation (6.5b)

ε_2 is selected via equation (6.5a).

The components (C.3) must be resolved into the global coordinate asystem. The coordinate system directed along $\underset{\sim}{g}$ must be successively rotated through the angles θ_5, θ_4, θ_3 and θ_2 and each

rotation θ_n alters only the two Cartesian components x_n and x_{n-1}. The complete transformation is

$$\underset{\sim}{v} = R''' R'' R' R\underset{\sim}{x} \tag{C.4}$$

where

$$R = \begin{bmatrix} \cos\theta_5 & -\sin\theta_5 & 0 & 0 & 0 \\ \sin\theta_5 & \cos\theta_5 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

$$R' = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & \cos\theta_4 & -\sin\theta_4 & 0 & 0 \\ 0 & \sin\theta_4 & \cos\theta_4 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

$$R'' = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & \cos\theta_3 & -\sin\theta_3 & 0 \\ 0 & 0 & \sin\theta_3 & \cos\theta_3 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

$$R''' = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & \cos\theta_2 & -\sin\theta_2 \\ 0 & 0 & 0 & \sin\theta_2 & \cos\theta_2 \end{bmatrix}$$

The angles θ_5 to θ_2 are just the hyper cylindrical coordinates of g relative to the global reference frame. The elements of the rotation matrices are

$$\cos\theta_5 = g_5/G_5 \quad \sin\theta_5 = G_4/G_5$$
$$\cos\theta_4 = g_4/G_4 \quad \sin\theta_4 = G_3/G_4$$
$$\cos\theta_3 = g_3/G_3 \quad \sin\theta_3 = G_2/G_3$$
$$\cos\theta_2 = g_2/G_2 \quad \sin\theta_2 = G_1/G_2$$

where

$$G_n = \left[\sum_{j=1}^{n} g_j^2 \right]^{\frac{1}{2}}$$

and the g_j are the global Cartesian coordinates of g. Substituting equation (C.3) for $\underset{\sim}{x}$ into (C.4) gives expressions for the components of $\underset{\sim}{g}'$ and equation (6.6) then defines the post-collision state of each particle. Notice that the deflection angle in three space and the energy exchange are intricately connected in this collision model.

It is probably more useful to separate the energy exchange and the deflection calculation so that any scattering in 3 space may be used. This is easily done by retaining only the rows of the matrix equation (C.4) which correspond to the two components of internal energy. These are

$$\begin{aligned} g_5' &= g_5 \cos\theta_5 - G_4 \sin\theta_5 \cos\theta_5 \\ g_4' &= g_4(\cos\theta_5 + g_5 \sin\theta_5 \cos\theta_4/G_4) \\ &\quad - G_5 G_3 \sin\theta_5 \sin\theta_4 \cos\theta_3/G_4 \ . \end{aligned} \qquad \text{(C.5)}$$

The three components of translational relative velocity (g_3', g_2', g_1') can be calculated in the normal way for any deflection angle in 3 space.

$$\cos\theta_5 = g_5/G_5 \quad \sin\theta_5 = G_4/G_5$$
$$\cos\theta_4 = g_4/G_4 \quad \sin\theta_4 = G_3/G_4$$
$$\cos\theta_3 = g_3/G_3 \quad \sin\theta_3 = G_2/G_3$$
$$\cos\theta_2 = g_2/G_2 \quad \sin\theta_2 = G_1/G_2$$

where

$$G_n = \left[\sum_{j=1}^{n} g_j^2 \right]^{\frac{1}{2}}$$

and the g_j are the global Cartesian coordinates of g. Substituting equation (C.3) for $\underset{\sim}{x}$ into (C.4) gives expressions for the components of $\underset{\sim}{g}'$ and equation (6.6) then defines the post-collision state of each particle. Notice that the deflection angle in three space and the energy exchange are intricately connected in this collision model.

It is probably more useful to separate the energy exchange and the deflection calculation so that any scattering in 3 space may be used. This is easily done by retaining only the rows of the matrix equation (C.4) which correspond to the two components of internal energy. These are

$$g_5' = g_5 \cos\theta_5 - G_4 \sin\theta_5 \cos\theta_5$$
$$g_4' = g_4(\cos\theta_5 + g_5 \sin\theta_5 \cos\theta_4/G_4) - G_5 G_3 \sin\theta_5 \sin\theta_4 \cos\theta_3/G_4 . \qquad (C.5)$$

The three components of translational relative velocity (g_3', g_2', g_1') can be calculated in the normal way for any deflection angle in 3 space.

14/4/02 mm!

```
% cos(t5) = g5/G5 sin(t5) = G4/G5
v1 = g5/G5*cos(chi) - G4/G5*sin(chi)*cos(eps4)
v2 = g4/G4*G4/G5*cos(chi) + ...
     g4/G4*g5/G5*sin(chi)*cos(eps4) - ...
     G3/G4*sin(chi)*sin(eps4)*cos(eps3)

gstar = G5*[ v1; v2 ]; % note that G5 = g
gstar = simple(gstar);

gstar(1) % = g5*cos(chi) - G4*sin(chi)*cos(eps4), see eqn C.5 in thesis
gstar(2) % = g4*cos(chi) +
         %       g4/G4*g5*sin(chi)*cos(eps4) -
         %            G5*G3/G4*sin(chi)*sin(eps4)*cos(eps3), see enq C.5
```

APPENDIX D

EXECUTION TIMES OF EXCHANGE MODELS

The execution speeds for the 5-space (5-S) collision models and Borgnakke and Larsen's (B+L) statistical exchange schemes were measured on two machines. The CDC FORTRAN (FTN5) compiler has various levels of optimisation from OPT=0 (no optimisation) to OPT=3 (maximum optimisation). The following versions of the compiler were used:

a) The ICCC batch system with OPT=0. With no optimisation the relative speeds might be similiar to that for a mini computer.

b) The ICCC time sharing system with (OPT=2). This is a representative type of compiler: DO loops are quick and the registers are extensively used so that intermediate results are not stored in memory. The machine itself is rather slow.

c) The ULCC 7600 batch processing system with the FTN5 compiler. There was no difference in speed between the second (OPT=2) and third (OPT=3) optimising levels.

Compiler (a) was only tested for the completely inelastic collision. Borgnakke and Larsen's method was 1.31 times faster than the 5-space collision model. This is presumably because of the time needed to calculate with an extra variable representing internal energy. In addition the DO loops in the 5-space model make it slower for this compiler than the B+L model for which explicit expressions for each of the three velocity components are written. The optimising compilers will reduce this penalty and the length of these DO loops (five iterations) is about that where it is better to use loops rather

than explicit expressions.

The execution times include only the basic calculation of the collision and not the time consuming collision selection procedures. Collisions between the same two particles were calculated a large number of times (1000 - 50000). Energy was conserved (to less than .004 % deviation) in all tests. Each execution speed, expressed as collisions/CPU seconds, was derived from at least three and usually more than 5 different tests. There was very little difference in the execution times for the runs which differed in the sequence of random numbers used. In the B+L scheme a randomly distributed beta variable must be chosen for each collision. The method is the acceptance - rejection technique and is given in the appendix of I.C. Aero Report (75-10) (Pullin 1975). To reduce the iterations the maximum value of the random variable must be known and is calculated from the indices of the beta distribution. Wherever possible this maximum is calculated once only. All calculations with the B+L schemes were for two internal degrees of freedom.

Table D.1

Execution speeds for exchange schemes-compilers (b) and (c).

	two class scheme		restricted exchange			
	$\phi = 1$		constant ϕ		variable-ϕ	
Model	(b)	(c)	(b)	(c)	(b)	(c)
B+L	1480	26480	1480	26480	1087	14520
5-S	1920	28240	1215	17600	1215	17600

Notes: For the constant ϕ calculations the speeds of each model have been deduced from other cases. For the B+L model the speed is virtually the same as for the completely inelastic collisions and should differ only because a random number is selected from a different distribution. For the 5-S model the execution time should be virtually the same as for variable-ϕ except for the time required to calculate the different value of ϕ for each collision.

The Borgnakke and Larsen restricted exchange scheme suffers with variable-ϕ since the indices of the beta distribution are not known in advance but are different for every collision. The maximum of the beta distribution is a function involving powers of the fractional indices . This maximum value must be calculated for each collision and this is a time-consuming operation. A step function for $\phi(e_{cm})$ might be used to reduce the computing time for the B+L variable-ϕ calculations. In this case the maximum of the beta variable for each ϕ could be calculated once only. This 'step variable-ϕ' calculation should execute nearly as fast as the constant ϕ calculations.

When used in simulations the number of collisions calculated per CPU second is less than that given above since the time for moving the particles and selecting collision pairs must be included. For the relatively simple one-dimensional shock the collision rate was 8000 - 13000 colls/CPU sec for compiler (c). For two-dimensional calculations the execution rate depends on the geometry, the Knudsen number and the various ratios of the moving, sampling and printing intervals. The rate is reduced to 1500 - 4000 colls/CPU sec

REFERENCES

Alder, B.J. and T. Wainwright (1958): 'Studies in Molecular Dynamics I. General Method', J. Chem. Phys., 31, p. 459

Alsmeyer, H. (1976): 'Density Profiles in Argon and Nitrogen Shock Waves Measured by the Absorption of an Electron Beam', J. Fluid Mech., 74, p.497

Annis, B. K. and A. P. Malinauskas (1971): 'Temperature Dependence of Rotational Collision Numbers from Thermal Transpiration', J. Chem. Phys., 54, p. 4763

Belotserkovskiy, O. M. and V. Y. Yanitsky (1978): 'Statistical Modelling of Flows of Ideal Monatomic Gases', Fluid Mech. Soviet Res., 7, p. 42

Bhatnagar, P. L. , E. P. Gross and M. Krook (1954): 'A Model for Collision Processes in Gases I. Small Amplitude Processes in Charged and Neutral One-Component Systems', Phys. Rev., 94, p. 511

Bird, G. A. (1963): 'Approach to Translational Equilibrium in a Rigid Sphere Gas', Phys. Fluids, 6, p. 1518, Academic Press

Bird, G. A. (1965): 'Shock Wave Structure in a Rigid Sphere Gas', Rarefied Gas Dynamics, 4th. Symposium (ed. de Leeuw), part I, p. 216

Bird, G. A. (1969): 'Direct Simulation Monte Carlo Method', Rarefied Gas Dynamics, 6th. Symposium (ed. Trilling & Wachman), part I, p. 85, Academic Press

Bird, G. A. (1970a): 'Aspects of the Structure of Strong Shock Waves', Phys. Fluids, 13, p. 1172

Bird, G. A. (1970b): 'Direct Simulation and the Boltzmann Equation', Phys. Fluids, 13, p. 2676

Bird, G. A. (1970c): 'Breakdown of Translational and Rotational Equilibrium in Gaseous Expansions', A.I.A.A. Jour., 8, p. 1998

Bird, G. A. (1973): 'Near Continuum Impact of an Underexpanded Jet Plume on a Wall', Proc. A.I.A.A Computational Fluid Dynamics Conf. 1973, p. 103

Bird, G. A. (1976): 'Molecular Gas Dynamics', Clarendon Press, Oxford

Bird, G. A. (1979): 'Simulation of Multi-Dimensional and Chemically Reacting Flows', Rarefied Gas Dynamics , 11th Symposium, (ed. Campragué), part I, p. 365, C.E.A. (Paris)

Bird, G. A. (1981): 'Monte-Carlo Simulation in an Engineering Context', Rarefied Gas Dynamics (ed. Fisher), 12th. Symposium, Part I, p. 239, (Progress in Astronautics and Aeronautics, 74, A.I.A.A)

Bird, G. A. (1983): 'Rarefied Hypersonic Flow Past a Slender Cone', to be published in Rarefied Gas Dynamics, 13th. Symposium

Borgnakke, C. and P. S. Larsen (1973): 'Statistical Collision Model for Monte-Carlo Simulation of Polyatomic Gas', Dept. of Fluid Mechanics, Technical University of Denmark, Lyngby, Denmark, AFM 73-08

Borgnakke, C. and P. S. Larsen (1975): 'Statistical Collision Model for Monte-Carlo Simulation of Polyatomic Gas Mixture', J. Comp. Phys., 18, p. 405

Brau, C. A. and R. M. Jonkman (1970): 'Classical Theory of Rotational Relaxation in Diatomic Gases', J. Chem. Phys., 52, p. 477

Butherus, T. F. and T. S. Storvick (1974): 'Rotational Collision Numbers and the Heat Conductivity of Nitrogen Gas from Thermal Transpiration Measurements to 1250 K', J. Chem. Phys., 60, p. 321

Carnevale, E. H., C. Cary and G. Larsen (1967): 'Ultrasonic Determination of Rotational Collision Numbers and Vibrational Relaxation Times of Polyatomic Gases at High Temperatures', J. Chem. Phys., 47, No. 8, p. 2829

Chahine, M. T. (1963): 'The Shock Structure According to the Krook Collision Model', Rarefied Gas Dynamics (ed. Laurmann), 3rd. Symposium, Part I, p. 260, Academic Press

Chapman, S. and T. G. Cowling (1952): 'The Mathematical Theory of Non-Uniform Gases', 2nd edn., (3rd edn. 1970), Cambridge University Press

Cheng, H. K. (1961): 'Hypersonic Shock-Layer Theory of the Stagnation Region at Low Reynolds Number', Proc. of the 1961 Heat Transfer and Fluid Mechanics Institute

Coleman, G. T., S. C. Metcalf and C. J. Berry (1977): 'Heat transfer to Hemishere Cylinders and Bluff Cylinders Between Continuum and Free Molecular Limits', Rarefied Gas Dynamics, 10th Symposium (ed. Potter), part I, p. 393, (Progress in Astronautics and Aeronautics, 51, A.I.A.A)

Cowling, T. G. (1950): 'Molecules in Motion', Hutchinson's University Library

Dahlen, G. A. and C. L. Brundin (1983): 'Wall Temperature Effects on Rarefied Hypersonic Cone Drag', to be published in Rarefied Gas Dynamics, 13th. Symposium

Davis, J. (1978): 'An Experimental Study to Evaluate and Develop the Direct Simulation Method as Applied to Rarefied Hypersonic Flow Fields', Dept. of Aero., Imperial College, Ph. D. Thesis

Davis, J., R. G. Dominy, J. K. Harvey, and M. N. Macrossan (1983): 'The Evaluation of Some Collision Models Used for the Monte-Carlo Calculation of Rarefied Hypersonic Flows', J. Fluid Mech., 135, p. 355

Dayman, B. (1965): 'Hypersonic Viscous Effects on Free-Flight Slender Cones', A.I.A.A. Jour., 3, p. 1391

Deiwert, G.S. and K. K. Yoshikawa (1975): 'Analysis of a Semi-Classical Model for Rotational Transition Probabilities', Phys. Fluids, 18, p. 1085

Deshpande, S. M., P. V. Subba Raju and N. Ramani (1979): 'A Comparative Study of the Time Counter and Random Collision Number Strategies Used in Monte Carlo Simulation', Rarefied Gas Dynamics, 11th Symposium (ed. Campragué), part I, p. 435, C.E.A. (Paris)

Dolman, K. A. (1980): 'Heat Transfer to a Hemisphere-Cylinder and a Bluff Cylinder in High Altitude Flight', R.A.E., Tech. Memo. Aero. 1819

Dominy, R. G., M. N. Macrossan and J. K. Harvey (1981): 'Rarefied Hypersonic Flow about a Blunt-Ended Circular Cylinder', Dept. of Aero., Imperial College, Rep. No. 81-01

Erofeev, A. I., and V. A. Perepukhov (1979): 'Hypersonic Rarefied Flow about a Flat Plate by the Direct Simulation Method', Rarefied Gas Dynamics, 11th Symposium (ed. Campragué), Part I, p. 417, C.E.A. (Paris)

Geiger, R. E. (1969): 'Slender Cone, Zero Angle of Attack Drag in Continuum and Non-Continuum Flow', A.I.A.A. paper 69-711

Hamel, B. B. and A. L. Cooper (1969): 'A First Collision Theory of the Hyperthermal Leading Edge Problem', Rarefied Gas Dynamics, 6th. Symposium (ed. Trilling & Wachman), part I, p. 443, Academic Press

Harvey, J. K., R. W. Jeffery and D. C. Uppington (1971): 'The Imperial College Graphite Heated Hypersonic Wind Tunnel', British A.R.C., R. & M. 3701

Haslam-Jones, T. F. (1978): 'Measurements of the Drag of Slender Cones in Hypersonic Flow at Low Reynolds Numbers Using a Magnetic Suspension and Balance', Dept. of Eng. Sci., Univ. of Oxford, Rep. No. 1235/78

Haviland, J. K. (1963): 'Determination of Shock-Wave Thickness by the Monte Carlo Method', Rarefied Gas Dynamics (ed. Laurmann), 3rd. Symposium, Part I, p. 274, Academic Press

Herzfeld K. F. and T. A. Litovitz (1959): 'Absorption and dispersion of Ultrasonic Waves', Academic Press

Hickman, R. S. (1967): 'An Experimental Study of a Hypersonic Rarefied Flow over a 10° Cone', Rarefied Gas Dynamics, 5th. Symposium (ed. Brundin), Part II, p. 1067, Academic Press

Hirschfelder, J. O., C. F. Curtiss and R. B. Bird (1954): 'Molecular Theory of Gases and Liquids', (2nd. edn. 1965), Wiley

Huang, K. (1963): 'Statistical Mechanics', Wiley

Hui, W. H. (1975): 'Simple Formulae for Supersonic Flow Past a Cone', Aeronautical Quarterly, 26, p. 11

Itikawa, Y. and K. K. Yoshikawa (1975): 'Monte-Carlo Calculations of Diatomic Molecule Gas Flows', NASA, Ames Research Centre, TND, 8100

Jeffery, R. W. (1975): 'The Aerodynamics of Wings in Low-Density Hypersonic Flow', Dept. of Aero., Imperial College, Ph. D. thesis

Keel, A. G., L. G. Kraige, R. D. Passmore and R. N. Zapata (1971): 'Hypersonic Low Density Cone Drag', A.I.A.A. paper 71-133

Keeler, R. N., M. Van Theil and B. J. Alder (1965): 'Corresponding States at Small Interatomic Distances', Physica, 31, p. 1437

Krook, M. and T. T. Wu (1977): 'Exact Solution of the Boltzmann Equation', Phys. Fluids, 20, p. 1589

Krylov, V. I. (1962): 'Approximate Calculation of Integrals', Macmillian

Larsen, P. I. and C. Borgnakke (1974): 'Statistical Collision Model for Simulating Polyatomic Gas with Restricted Energy Exchange', Rarefied Gas Dynamics, 9th Symposium (ed. Becker & Fiebig), paper A7, DFVLR Press (Göttingen)

Larsen, P. I. (1976): 'Monte Carlo Simulation of a Homogeneous Dissociating Gas', Arch. Mech., 28, p. 719

Liepman H. W., R. Narasimha and M. T. Chahine (1962): 'Structure of a Plane Shock Layer', Phys. Fluids, 5, p. 1313, (for errata see 8, p. 551)

Liepman H. W. and A. Roshko (1957): 'Elements of Gasdynamics', Wiley

Lengrand, J-C, and M. Raffin and J. Allègre (1981): 'Monte Carlo Simulation Method Applied to Jet Wall Interactions under Continuum Flow Conditions', Rarefied Gas Dynamics (ed. Fisher), 12th. Symposium, Part II, p. 994, (Progress in Astronautics and Aeronautics, 74, A.I.A.A)

Lordi, J. A. and R. E. Mates (1970): 'Rotational Relaxation in Nonpolar Diatomic Gases', Phys. Fluids, 13, No. 2, P. 291

Macpherson, A. K. (1969): 'Shock Collision at a Molecular Level', J. Fluid Mech., 39, p. 849

Macpherson, A. K. (1971): 'Rotational Temperature Profiles of Shock Waves in Diatomic Gases', J. Fluid Mech., 49, Part 2, p. 337

Macrossan, M. N. (1981): 'Improvements of the Algorithms Used for Monte-Carlo Direct Simulation Computations', Dept. of Aero., Imperial College, Rep. No. 81-03

Melville, W. K. (1972): 'The Use of the Loaded Sphere Molecular Model for Computer Simulation of Diatomic Gases', J. Fluid. Mech., 51, p. 571

Merkle, C. L., H. W. Behrens and R. D. Hughes (1981): 'Application of the Monte Carlo Simulation Procedure in the Near Continuum Regime', Rarefied Gas Dynamics (ed. Fisher), 12th. Symposium, Part I, p. 256, (Progress in Astronautics and Aeronautics, 74, A.I.A.A)

Metcalf, S. C., G. T. Coleman and C. J. Berry (1974): 'Heat Transfer to Bluff Faced and Hemispherical Faced Cylinders between Continuum and Free Molecular Limits', Rarefied Gas Dynamics, 9th Symposium (ed. Becker & Fiebig), paper D16, DFVLR Press (Gottingen)

Monchick, L. and E. A. Mason (1961): 'Transport Properties of Polar Gases', J. Chem. Phys., 35, No. 5, p. 1676

Morse, P. M. (1929): 'Diatomic Molecules According to the Wave Mechanics II. Vibrational Levels', Phys. Rev., 34, p. 51

Mott-Smith, H. M. (1951): 'The Solution of the Boltzmann Equation for a Strong Shock Wave', Phys. Rev., 82, p. 885.

Muckenfuss, C. (1962): 'Some Aspects of Shock Structure According to the Bimodal Model', Phys. Fluids, 5, p. 1325

Nanbu, K. (1980a): 'Direct Simulation Scheme Derived from the Boltzmann Equation. I. Monocomponent Gases', J. Phys. Soc. Japan, 49, p. 2042

Nanbu, K. (1980b): 'Direct Simulation Scheme Derived from the Boltzmann Equation. II. Multicomponent Gas Mixtures', J. Phys. Soc. Japan, 49, p. 2050

Nanbu, K. (1980c): 'Direct Simulation Scheme Derived from the Boltzmann Equation. III. Rough Sphere Gases', J. Phys. Soc. Japan, 49, p. 2055

Nanbu, K. (1981a): 'Direct Simulation Scheme Derived from the Boltzmann Equation. IV. Correlation of Velocity', J. Phys. Soc. Japan, 50, p. 2829

Nanbu, K. (1981b): 'Slowing Down of Energetic Molecules in a Spatially Uniform Gas', Rep. Inst. High Speed Mech., Tohoku Univ., Japan, 43, Rep. No. 335

Nanbu, K. (1982a): 'Direct Simulation Scheme Derived from the Boltzmann Equation. V. Effects of Sample Size, Number of Molecules, Step Size, and Cut-Off Angle upon Simulation Data', Rep. Inst. High Speed Mech., Tohoku Univ., Japan, 45, Rep. No. 348

Nanbu, K. (1982b): 'Direct Simulation Scheme Derived from the Boltzmann Equation. VI. Velocity Correlation in a Model Cell', J. Phys. Soc. Japan, 51, p. 59

Nanbu, K. (1982c): 'Direct Simulation Scheme Derived from the Boltzmann Equation. VIII. Velocity Correlation Relevant to Boundary Conditions', J. Phys. Soc. Japan, 51, p. 1763

Nanbu, K. (1982d): 'Applicability of the Random Walk Model to Free Molecular Motion in the Direct Simulation Method', Rep. Inst. High Speed Mech., Tohoku Univ., Japan, 45, Rep. No. 350

Nanbu, K. and Y. Watanabe (1981): 'Relaxation Rates of Inverse-Power and Rigid-Sphere Molecules', Rep. Inst. High Speed Mech., Tohoku Univ., Japan, 43, Rep. No. 334

Neyland, C. (1967): 'Rotational Relaxation of Homonuclear Diatomic Molecules', J. Chem. Phys., 46, p. 63

Nordsieck, A. and B. L. Hicks (1967): 'Monte Carlo Evaluation of the Boltzmann Collision Integral', Rarefied Gas Dynamics, 5th. Symposium (ed. Brundin), Part I, p. 695, Academic Press

Parker, J. G. (1959): 'Rotational and Vibrational Relaxation in Diatomic Gases', Phys. Fluids, 2, p. 449

Pearson, W. E. and C. F. Hansen (1974): 'Collision Induced Rotational Transition Probabilities', Rarefied Gas Dynamics, 8th Symposium (ed. Karamcheti), p. 167, Academic Press

Potter, J. L. (1967): 'The Transitional Rarefied-Flow Regime', Rarefied Gas Dynamics, 5th. Symposium (ed. Brundin), Part II, p. 881, Academic Press

Pullin, D. I. (1974): 'Rarefied Leading Edge Flow of a Diatomic Gas', Dept. of Aero., Imperial College, Ph.D. Thesis

Pullin, D. I. (1975): 'Model Kinetic Equations for Structureless Polyatomic Molecules with Phenomenological Energy Exchange', Dept. of Aero, Imperial College, Rep. No. 75-10

Pullin, D. I. (1978): 'Kinetic Models for Polyatomic Molecules with Phenomenological Energy Exchange', Phys. Fluids, 21, p. 209

Pullin, D. I. (1980): 'Direct Simulation Methods for Compressible Inviscid Ideal-Gas Flow', J. Comp. Phys., 34, p. 231

Pullin, D. I., J. Davis and J. K. Harvey (1977): 'Monte-Carlo Calculations of the Rarefied Transition Flow Past a Bluff Faced Cylinder', Rarefied Gas Dynamics, 10th Symposium (ed. Potter), part I, p. 379, (Progress in Astronautics and Aeronautics, 51, A.I.A.A)

Pullin, D. I. and J. K. Harvey (1976): 'A Numerical Simulation of the Rarefied Hypersonic Flat-Plate Problem', J. Fluid Mech., 78, p. 689

Robben, F. and L. Talbot (1966a): 'Measurements of Shock Wave Thickness by the Electron Beam Fluorescence Method', Phys. Fluids, 9, p. 633

Robben, F. and L. Talbot (1966b): 'Measurements of the Rotational Distribution Function of Nitrogen in a Shock Wave', Phys. Fluids, 9, p. 653

Schmidt, B. (1969): 'Electron Beam Density Measurements in Shock Waves', J. Fluid Mech., 39, 36

Sturtevant, B. and E. A. Steinhilper (1974): 'Intermolecular Potentials from Shock Structure Experiments', Rarefied Gas Dynamics, 8th Symposium (ed. Karamcheti), p. 159, Academic Press

Tolman, R. C. (1938): 'The principles of Statistical Mechanics', Oxford University Press

Vincenti, W. G. and C. H. Kruger (1965): 'An Introduction to Physical Gas Dynamics', Wiley, New York

Vinokur, M. (1959): 'Hypersonic Flow Around Bodies of Revolution which are Generated by Conic Sections', 6th. Midwestern Conferenec on Fluid Mechanics, University of Texas

Vinokur, M. (1962): 'Laminar Heat-Transfer Distribution on Oblate Ellipsoidal Noses in Hypersonic Flow', J. Aerosp. Sci., 29, p. 113

Watanabe, Y. and K. Nanbu (1982): 'Direct Simulation Scheme Derived from the Boltzmann Equation. VII. Ergodicity of Simulation Solutions', Rep. Inst. High Speed Mech., Tohoku Univ., 45, Rep. No. 349

Whitfield, D. L. (1973): 'Mean Free Path of Emitted Molecules and Correlation of Sphere Drag Data', A.I.A.A. Jour., 11, p. 1666

Wooley, H. W. (1956): 'Thermodynamic Properties of Gaseous Nitrogen', NACA TN 3271

Wu, T-Y and T. Ohmura (1962): 'The Quantum Theory of Scattering', Prentice-Hall

Yen, S. M., F. G. Tcheremissine (1981): 'Monte-Carlo Solutions of the Nonlinear Boltzmann Equation', Rarefied Gas Dynamics, 12th. Symposium (ed. Fisher), Part I, p. 287, (Progress in Astronautics and Aeronautics, 74, A.I.A.A)

Yen, S. M., W. P. Walters, W. Ng and J. R. Flood (1974): 'Solutions of the Non-Linear Boltzmann Equation for Shock Waves in a Maxwellian Gas', Rarefied Gas Dynamics, 8th Symposium (ed. Karamcheti), p. 137, Academic Press